**LISTING OF CLAIMS**

This listing of claims will replace all prior versions, and listings, of claims in this application.

1. (withdrawn) A crystallizable composition comprising

a) a purified enzyme selected from unphosphorylated JNK1, unphosphorylated JNK2, unphosphorylated JNK3, or an unphosphorylated isoform of said enzyme, wherein said enzyme contains a C-terminal deletion of about 20 amino acids and, if said enzyme is unphosphorylated JNK3, said enzyme additionally contains an N-terminal deletion of about 40 amino acids;

b) a non-hydrolyzable ATP analog or a suicidal substrate;

c) magnesium ions;

d) between about 10 to 30% v/v polyethylene glycol monomethyl ether;

e) between about 5 to 20% v/v ethylene glycol;

f) a reducing agent at a final concentration of between about 5 to 50 mM; and

g) a buffer that maintains pH at between about 7.0 and 7.5.

2. (withdrawn) The crystallizable composition according to claim 1, wherein said unphosphorylated JNK3 enzyme is JNK3 1.

3. (withdrawn) The composition according to claims 1 or 2, wherein said non-hydrolyzable ATP analog is AMP-PNP.

4. (withdrawn) A crystallized complex capable of being resolved at 2.3 Å resolution comprising:

a) a purified enzyme selected from unphosphorylated JNK1, unphosphorylated JNK2, unphosphorylated JNK3, or an unphosphorylated isoform of said enzyme, wherein said enzyme contains a C-terminal deletion of about 20 amino acids and, if said enzyme is unphosphorylated JNK3, said enzyme additionally contains an N-terminal deletion of about 40 amino acids;

b) a non-hydrolyzable ATP analog or a suicidal substrate; and

c) magnesium ions.

5. (withdrawn) The crystallized complex according to claim 4, wherein said unphosphorylated JNK3 enzyme is JNK3 1.

6. (withdrawn) The crystallized complex according to claim 4, wherein said non-hydrolyzable ATP analog is AMP-PNP.

7. (withdrawn) A method of obtaining a crystal comprising a purified enzyme selected from unphosphorylated JNK1, unphosphorylated JNK2, unphosphorylated JNK3, or an unphosphorylated isoform of said enzyme, said crystal being capable of being resolved at 2.3 Å resolution, comprising the step of subjecting a composition according to claims 1 or 2 to conditions which promote crystallization.

8. (withdrawn) A computer for producing a three-dimensional representation of:

a) a molecule or molecular complex, wherein said molecule or molecular complex comprises a binding pocket defined by structure coordinates of JNK3 amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Val78, Ala91, Lys93, Glu111, Ile124, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Gln155, Lys191, Ser193, Asn194, Val196 and Leu206, according to Figure 1; or

b) a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket

that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å,

wherein said computer comprises:

(i) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises the structure coordinates of JNK3 amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Val78, Ala91, Lys93, Glu111, Ile124, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Gln155, Lys191, Ser193, Asn194, Val196 and Leu206, according to Figure 1;

(ii) a working memory for storing instructions for processing said machine-readable data;

(iii) a central-processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine readable data into said three-dimensional representation; and

(iv) a display coupled to said central-processing unit for displaying said three-dimensional representation.

9. (withdrawn) The computer according to claim 8, wherein said computer produces a three-dimensional representation of:

a) a molecule or molecular complex comprising a binding pocket defined by the structure coordinates of JNK3 amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Ile77, Val78, Cys79, Ala80, Val90, Ala91, Ile92, Lys93, Lys94, Leu95, His104, Arg107, Glu111, Ile124, Ser125, Leu144, Val145, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Leu153, Cys154, Gln155, Asp189, Lys191, Pro192, Ser193, Asn194, Ile195, Val196 Val197, Lys204, Leu206 and Asp207, according to Figure 1; or

b) a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å; and

wherein said machine readable data comprises the structure coordinates of JNK3 amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Ile77, Val78, Cys79, Ala80, Val90, Ala91, Ile92, Lys93, Lys94, Leu95, His104, Arg107, Glu111, Ile124, Ser125, Leu144, Val145, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Leu153, Cys154, Gln155, Asp189, Lys191, Pro192, Ser193, Asn194, Ile195, Val196 Val197, Lys204, Leu206 and Asp207, according to Figure 1.

10. (withdrawn) The computer according to claims 8 or 9, wherein said computer produces a three-dimensional representation of:

a) a molecule or molecular complex defined by structure coordinates of JNK3 amino acids set forth in Figure 1; or

b) a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å; and

wherein said machine readable data contains the coordinates of JNK3 complex set forth in Figure 1.

11. (withdrawn) A computer for determining at least a portion of the structure coordinates corresponding to X-ray diffraction data obtained from a molecule or molecular complex, wherein said computer comprises:

a) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises at least a portion of the structural coordinates of the JNK3 complex according to Figure 1;

b) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises X-ray diffraction data obtained from said molecule or molecular complex;

c) a working memory for storing instructions for processing said machine-readable data of (a) and (b);

d) a central-processing unit coupled to said working memory and to said machine-readable data storage medium of (a) and (b) for performing a Fourier transform of the machine readable data of (a) and for processing said machine readable data of (b) into structure coordinates; and

e) a display coupled to said central-processing unit for displaying said structure coordinates of said molecule or molecular complex.

12. (withdrawn) A method for evaluating the potential of a chemical entity to associate with:

a) a molecule or molecular complex comprising a binding pocket defined by structure coordinates of JNK3 amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Val78, Ala91, Lys93, Glu111, Ile124, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Gln155, Lys191, Ser193, Asn194, Val196 and Leu206 according to Figure 1; or

b) a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å,

said method comprising the steps of:

(i) employing computational means to perform a fitting operation between the chemical entity and a binding pocket of the molecule or molecular complex; and

(ii) analyzing the results of said fitting operation to quantify the association between the chemical entity and the binding pocket; and

(iii) outputting said quantified association to a suitable output hardware.

13. (withdrawn) The method according to claim 12, wherein said method evaluates the potential of chemical entity to associate with:

a) a molecular or molecular complex comprising a binding pocket defined by the structural coordinates of JNK3 amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Ile77, Val78, Cys79, Ala80, Val90, Ala91, Ile92, Lys93, Lys94, Leu95, His104, Arg107, Glu111, Ile124, Ser125, Leu144, Val145, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152,

Leu153, Cys154, Gln155, Asp189, Lys191, Pro192, Ser193, Asn194, Ile195, Val196 Val197, Lys204, Leu206 and Asp207, according to Figure 1; or

b) a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

14. (withdrawn) The method according to claims 12 or 13, wherein said method evaluates the potential of a chemical entity to associate with a molecule or molecular complex:

a) defined by the set of structure coordinates for JNK3 amino acids, as set forth in Figure 1; or

b) a homologue of said molecule or molecular complex having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

15. (withdrawn) A method of obtaining structural information about a molecule or a molecular complex whose structure is unknown, comprising the steps of:

a) crystallizing said molecule or molecular complex of unknown structure;

b) generating an X-ray diffraction pattern from said crystallized molecule or molecular complex; and

c) applying at least a portion of the structure coordinates set forth in Figure 1 to the X-ray diffraction data to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown.

16. (currently amended) A method for identifying an inhibitor ~~potential agonist or antagonist~~ of an unphosphorylated JNK3 (c-Jun N-terminal kinase 3) ~~or a JNK3 mutant~~ molecule, comprising the step of:

~~wherein all or part of the~~ using all or part of a binding pocket of the unphosphorylated JNK3, which binding pocket comprises the atomic coordinates of amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Val78, Ala91, Lys93, Glu111, Ile124, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Gln155, Lys191, Ser193, Asn194, Val196 and Leu206 according to Figure 1A, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, ~~are determined to comprise a binding pocket in the JNK3 molecule or JNK3 mutant molecule to be used~~ to design or select said ~~potential agonist or antagonist,~~ inhibitor.

17. (currently amended) The method according to claim 16, wherein said binding pocket ~~all or part of the~~ additionally comprises the atomic coordinates of amino acids ~~Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76,~~ Ile77, ~~Val78,~~ Cys79, Ala80, Val90, ~~Ala91,~~ Ile92, ~~Lys93,~~ Lys94, Leu95, His104, Arg107, ~~Glu111, Ile124,~~ Ser125, Leu144, Val145, ~~Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152,~~ Leu153, Cys154, ~~Gln155,~~ Asp189, ~~Lys191,~~ Pro192, ~~Ser193, Asn194,~~ Ile195, ~~Val196,~~ Val197, Lys204~~, Leu206~~ and Asp207 according to Figure 1A, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å ~~are determined to comprise a binding pocket in a JNK3 (c-Jun N-terminal kinase 3) molecule or JNK3 mutant molecule~~.

18. (canceled)

19. (currently amended) The method according to claim 16 or 17, wherein the ~~potential agonist or antagonist~~ inhibitor is contacted with said unphosphorylated JNK3 (~~c-Jun N-terminal kinase 3)~~ molecule ~~or JNK3 mutant molecule~~ to determine the ability of said ~~potential agonist or antagonist~~ inhibitor to interact with the unphosphorylated JNK3 molecule ~~or JNK3 mutant molecule~~.

20. (currently amended) ~~The~~ A method for identifying an inhibitor of an unphosphorylated JNK3 (c-Jun N-terminal kinase 3) molecule ~~according to claim 16 or 17, further comprising, prior to step a),~~ comprising the steps of:

**[[i]]** a) producing a crystal of an unphosphorylated JNK3 (c-Jun N-terminal kinase 3) ~~or JNK3 mutant~~ molecule and a chemical entity, wherein said unphosphorylated JNK3 ~~or JNK3 mutant~~ molecule contains an N-terminal deletion of ~~about 40~~ 39 amino acids ~~and a C-terminal deletion of about 20 amino acids~~; ~~and~~

**[[ii]]** b) determining the three-dimensional atomic coordinates of amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Ile77, Val78, Cys79, Ala80, Val90, Ala91, Ile92, Lys93, Lys94, Leu95, His104, Arg107, Glu111, Ile124, Ser125, Leu144, Val145, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Leu153, Cys154, Gln155, Asp189, Lys191, Pro192, Ser193, Asn194, Ile195, Val196 Val197, Lys204, Leu206 and Asp207 of a binding pocket of the unphosphorylated JNK3 ~~or JNK3 mutant~~ molecule by X-ray diffraction of the crystal,

c) using all or part of said coordinates, ± a root mean square deviation from the backbone atoms of said amino

acids of not more than 1.5 Å, to design or select said inhibitor.

21. (currently amended) **[[A]]** The method according to claim 20, further comprising the step of ~~for identifying a potential agonist or antagonist of a JNK3 (c-Jun N-terminal kinase 3) or a JNK3 mutant molecule comprising the steps of:~~

~~a) producing a crystal of a JNK3 or JNK3 mutant molecule and a chemical entity, wherein said JNK3 or JNK3 mutant molecule contains an N-terminal deletion of about 40 amino acids and a C-terminal deletion of about 20 amino acids;~~

~~b) determining the three-dimensional atomic coordinates of the JNK3 or JNK3 mutant molecule by X-ray diffraction of the crystal;~~

~~c) using all or part of the atomic coordinates of the JNK3 or JNK3 mutant molecule to design or select said potential agonist or antagonist, wherein the atomic coordinates of the JNK3 or JNK3 mutant molecule are defined by Figure 1A ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å; and~~

~~d)~~ contacting said ~~potential agonist or antagonist~~ inhibitor with said unphosphorylated JNK3 ~~or JNK3 mutant~~ molecule to determine the ability of said ~~potential agonist or~~

~~antagonist~~ inhibitor to interact with said unphosphorylated JNK3 ~~or JNK3 mutant~~ molecule.

22. (new) The method according to claim 20, wherein said unphosphorylated JNK3 molecule further contains a C-terminal deletion of 20 amino acids.